PART 6

COMPARISON OF MODEL RESULTS

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6.1. Summary

Three levels of models were used or developed during the Lake Michigan Mass Balance Project (LMMBP). The toxic fate and transport/-bioaccumulation portion of the project included a previously-developed model (MICHTOX) for the coarse scale Level 1 and newly-developed models (LM2-Toxic and LM Food Chain) for the middle resolution Level 2. MICHTOX was used to assist in the development of the sampling program and to provide a screening-level assessment of the polychlorinated biphenyl (PCB) data. The LM2-Toxic and LM Food Chain models (LM models) were developed during the LMMBP as part of a suite of integrated mass balance models. While similar in function, the Level 1 and Level 2 models had different development histories and capabilities, and a comparison of model results was useful to evaluate suitability for potential future uses. This chapter provides an examination of the similarities and differences between the models and compares the results of scenario predictions from both sets of models.

The LM models provided a higher resolution evaluation of PCB dynamics on a spatial, chemical, and biological scale than MICHTOX. The higher resolution of the LM models included hydrodynamically modeled water transport, smaller water quality segments, congener versus homolog-level modeling, and a more detailed, data-based food web structure. While both sets of models used similar kinetics and forcing functions, the LM models were more fully calibrated to process data that were not available during the earlier development of the MICHTOX model. The higher resolution and more thorough calibration should allow the LM models to provide better representation of system processes and better predictions of the effects of future loading changes. These features of the LM models should also allow them to be used with minimal re-calibration for modeling localized areas of the lake that may have different congener composition, carbon production, or lake trout diets.

544

The comparison of model results demonstrated that, while differences in model parameterization resulted in different flux rates for important processes in PCB cycling in Lake Michigan, the annual net changes in water column concentrations were similar. The different flux rates resulted in different steady-state concentration predictions under a hypothetical constant loading condition scenario. However, under a scenario with declining loading trends based on scientific literature, predicted concentrations in water and fish from both sets of models converged and the rate of decline was more important to the model results than differences in model parameterization.

6.2 Comparison of Models

The LMMBP included three levels of models (Figure 6.1). For the PCB contaminant evaluation, MICHTOX represented the simpler, coarse resolution models. MICHTOX is comprised of two submodels: a toxics fate and transport submodel, and a food chain bioaccumulation submodel. LM2-Toxic and LM Food Chain (LM models) represented the higher resolution Level 2 models. This section discusses the similarities and differences in the models.

6.2.1 Model Similarities

The toxics models were similar in a number of ways. The MICHTOX fate and transport submodel and the LM2-Toxic model were both based upon the United States Environmental Protection Agency (USEPA) WASP4 toxics model (Ambrose *et al.*, 1988) and used similar approaches for modeling toxic fate and transport. While MICHTOX still possessed the general structure of WASP4, the LM2-Toxic computer code was completely new. MICHTOX and LM2-Toxic contained similar kinetics and mass transport functions. Both models included advection, dispersion, diffusion, settling and resuspension of toxics bound to particles, and deep sediment burial. The air/water exchange functions were also similar in the models. Both models used the 1994-1995 LMMBP data to develop forcing functions for tributary loads, atmospheric deposition, and atmospheric vapor concentrations, although LM2-Toxic simulated individual PCB congeners while MICHTOX simulated total PCBs divided into two homologs.
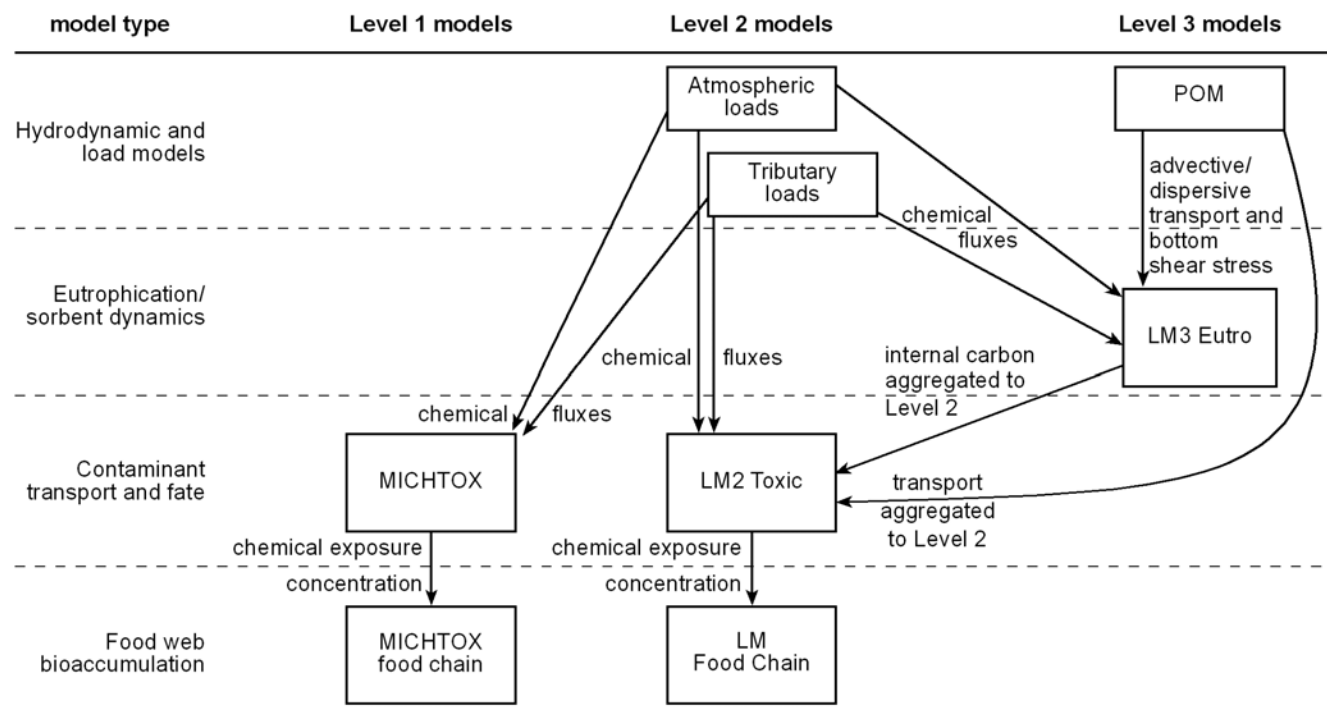

Figure 6.1. Supporting models and links for MICHTOX and the LM models.

The food chain bioaccumulation models were also conceptually similar. The MICHTOX food chain submodel and the LM Food Chain model were both based upon the concept of mass conservation and used similar kinetic processes, including uptake, elimination, and concentration reduction through growth. Both models used the LMMBP data set for estimates of fish and invertebrate weight, growth, and initial concentrations.

6.2.2 Model Differences

The primary differences in the models involved the level of resolution and the degree of calibration. The LM models provided a higher resolution evaluation of PCB dynamics with regard to spatial scales, hydrodynamic scales, kinetic processes, PCB forms, and biological components. The LM models were also rigorously calibrated using extensive field and process data, while MICHTOX was developed at a time when few PCB data were available.

LM2-Toxic was developed using a higher resolution spatial grid than MICHTOX; this provided a more accurate representation of spatially-dependent processes and of the effects of spatial variability in loads and concentrations. The LM2-Toxic water quality grid was composed of five vertical segments and 41 total water segments (Figure 4.3.1), while the MICHTOX grid used two vertical segments and nine total water segments (Figure 3.3.2). LM2-Toxic was also much more highly resolved in sediment segments having 53 sediment segments divided into non-depositional, transitional, and depositional zones (Figure 4.3.2). MICHTOX used six sediment segments (Figure 3.3.2), with the area of the segments adjusted to represent sediment focusing of contaminants.

The hydrodynamic processes in the models also used different resolutions. LM2-Toxic used hydrodynamic predictions from the fine-scaled (44,042 cell) Great Lakes version of the Princeton Ocean Model (GL-POM) aggregated to the 41-segment LM2-Toxic grid. Horizontal and vertical flows were obtained from the GL-POM hydrodynamic model and dispersion coefficients from the temperature model (see Section 4.5.1 in Part 4, Chapter 5 for details). MICHTOX used externally-specified estimates of advective and dispersive exchanges between its nine segments.

The LM models also contained higher resolution water quality kinetics and PCB forms. They simulated over 30 state variables (34 in LM2-Toxic, 40 in LM-Food Chain) representing PCB congeners or co-eluting congeners. MICHTOX modeled total PCBs in water, sediment, and the food web as two homologs. LM2-Toxic contained three carbon classes for partitioning of toxics: biotic carbon (BIC), particulate detrital carbon (PDC), and dissolved organic carbon (DOC). MICHTOX used a single solids class with a seasonally-specified fraction of organic carbon along with DOC. LM2-Toxic used dynamic phytoplankton carbon production loads estimated using the LM3-Eutro model, while MICHTOX carbon loads were based upon a steady-state solids balance and seasonal organic carbon fraction calculated from historical data.

In addition to containing more detail in PCB state variables, LM Food Chain was more detailed in its representation of the food chain than the MICHTOX food chain submodel. The LM Food Chain model was based on the LMMBP data and included phytoplankton, three invertebrates, and six fish species. The MICHTOX food chain submodel used an idealized food chain that included phytoplankton, two invertebrates, and two fish species.

The models also differ in the degree of calibration applied to them. LM2-Toxic and LM Food Chain were thoroughly calibrated to the LMMBP data set, and the LM2-Toxic was confirmed against a sediment core derived PCB hindcast loading estimate. In addition, the LM models had process data available to reduce degrees of freedom during calibration, such as particulate settling velocities, sediment mixing zone thicknesses, and complete fish diet data. MICHTOX was never fully calibrated against a PCB data set. It was calibrated to solids transport and plutonium data, validated to the small amount of PCB data available when the model was originally developed, and later compared to three hypothetical hindcast loading scenarios and the LMMBP data set (Endicott et al., 2005; Endicott, 2005). At the time of development of MICHTOX, there were little process data available against which to constrain the model parameterization.

6.3 Comparison of Model Results

6.3.1   Comparison of Mass Budget Analyses

Mass budget analyses were conducted for PCB simulation results for the 1994-1995 LMMBP sampling period from both the MICHTOX fate and transport submodel and LM2-Toxic (Part 3, Chapter 3, Section 3.3.3.3 and Part 4, Chapter 6, Section 4.6.2).   For this and the following comparisons, results from the LM models for individual congeners were summed and then converted to total PCB concentrations (Part 4, Chapter 6, Section 4.6.1) for comparison with results from the MICHTOX model.

There were a number of similarities in the results from both models. They both demonstrated a net loss of PCBs from the system. The net loss was calculated as the sum of fluxes out of the system minus the sum of fluxes into the system, or (sediment burial + gross volatilization + export to Lake Huron + Chicago diversion) - (tributary loads + atmospheric deposition + gas absorption + input from Lake Huron). Predicted net losses from the system were 2,673 kg/year for MICHTOX and 1,863 kg/year for the LM2-Toxic. The net loss from the system means that, under measured 1994-1995 loads, the system was not at steady-state and observed concentrations would decline. For the water column only, predicted net losses of total PCBs were similar for both models: 182 kg/year for MICHTOX and 159 kg/year for LM2-Toxic.

Both models show that gross volatilization, gas absorption, resuspension, and settling are significant mass transfer rate processes in the Lake Michigan system (Figure 6.2). Net volatilization of PCBs was the largest flux process. Resuspension of PCBs was greater than settling for both models, which means there was a net movement of PCBs from the sediment to the water column. Export of PCBs to Lake Huron or through the Chicago diversion was negligible, and was not shown on Figure 6.2.

The results in Figure 6.2 highlight the differences in parameterization of the models. PCB resuspension and settling fluxes were much greater for MICHTOX than for LM2-Toxic. Volatilization and gas absorption fluxes were also higher in MICHTOX. MICHTOX was
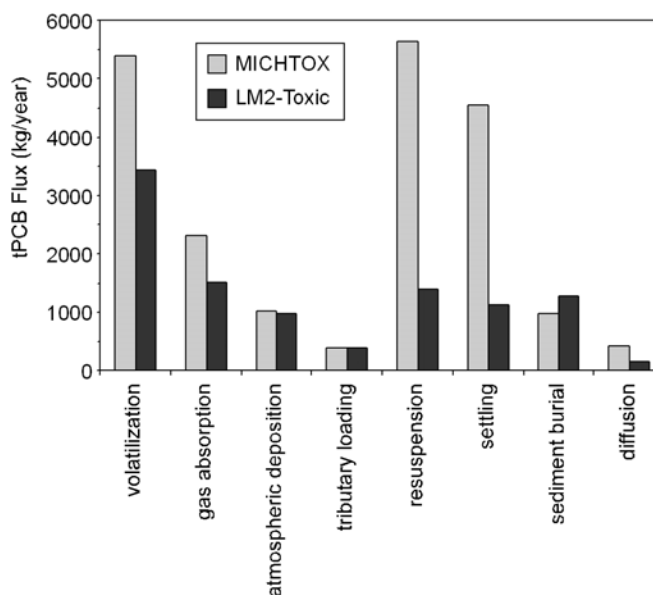

Figure 6.2. Comparison of the Lake Michigan total PCB mass balance analyses results, 1994-1995.

predicting more PCBs moving from the sediment to the water column than LM2-Toxic through net resuspension and diffusion, but was also removing more PCBs from the water column through net volatilization. This resulted in the net change in PCB mass in the water column being similar between the models. Net resuspension fluxes and diffusion in MICHTOX were as large of a PCB source to the water column as the external loads. They were less than a third of the external loads for the LM2-Toxic. LM2-Toxic has a greater sediment burial loss from the system, but the magnitude is small compared to net volatilization losses.

6.3.2   Comparison of Model Forecast Scenarios

Results for the model forecast scenarios were compared from both the fate and transport models and the food chain/bioaccumulation models. For comparison purposes, the LM2-Toxic segment results were volume-weighted and averaged to match the MICHTOX segmentation.   The bioaccumulation model results provided only an approximate comparison between models because the MICHTOX food chain submodel lake trout concentrations were modeled on a segment-wide

547

basis and the LM Food Chain results were for the biota boxes used for model calibration.

A comparison of the Constant Conditions Scenario results showed that MICHTOX predicted lower concentrations in the epilimnion than LM2-Toxic (Figure 6.3). This agreed with the model comparison to 1994-1995 data in which MICHTOX underpredicted epilimnion concentrations (Part 4, Chapter 3). The models contained the same general processes and used the same forcing functions, therefore, differences in predicted concentrations were primarily due to model parameterization and resolution differences. For the southern Lake Michigan model segments, hypolimnetic concentrations reached comparable concentrations at steady-state even though MICHTOX had higher annual average concentrations initially. While both models used the same initial conditions, MICHTOX had higher sediment PCB resuspension rates which resulted in the higher initial annual average

hypolimnetic water column concentrations shown on the plot. For the central Lake Michigan hypolimnetic segments, MICHTOX predicted lower concentrations than LM2-Toxic.

Sediment concentration predictions were slightly higher for MICHTOX than for the LM2-Toxic model (Figure 6.4). The initial sediment concentrations on a ng/L basis were significantly different between the models. While both models used initial conditions based upon measured 1994-1995 PCB concentrations (ng PCB/g sediment), LM2-Toxic also used measured porosity from the 1994-1995 data while MICHTOX used the same porosity and sediment density used during the initial model development.

The water concentration results from the Continued Recovery – Fast Scenario were also compared (Figure 6.5). For both sections of Lake Michigan,
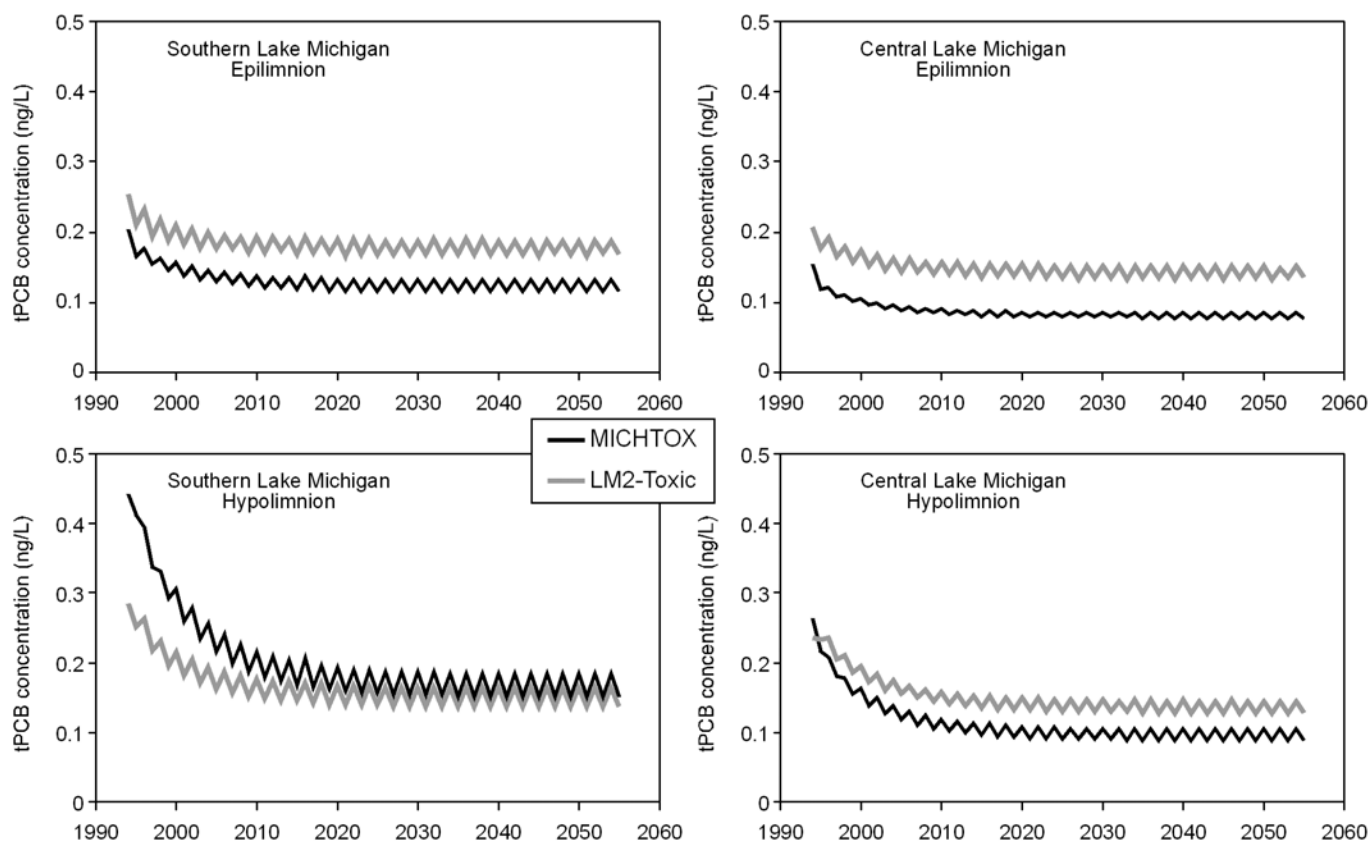

Figure 6.3. Comparison of model output annual average total PCB water concentrations for the Constant Conditions Scenario.
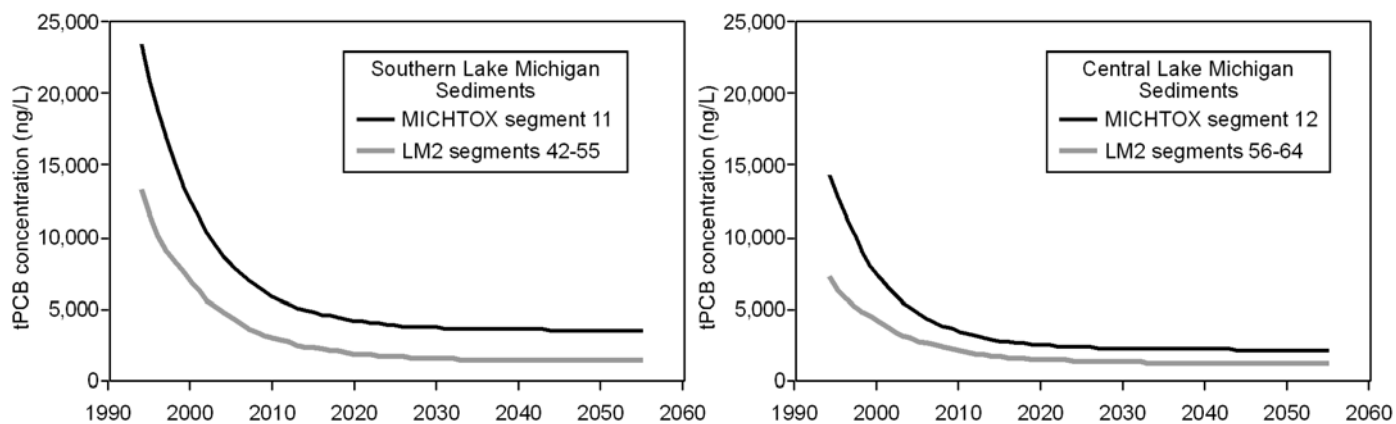
Figure 6.4. Comparison of model output annual average total PCB sediment concentrations for the Constant Conditions Scenario.
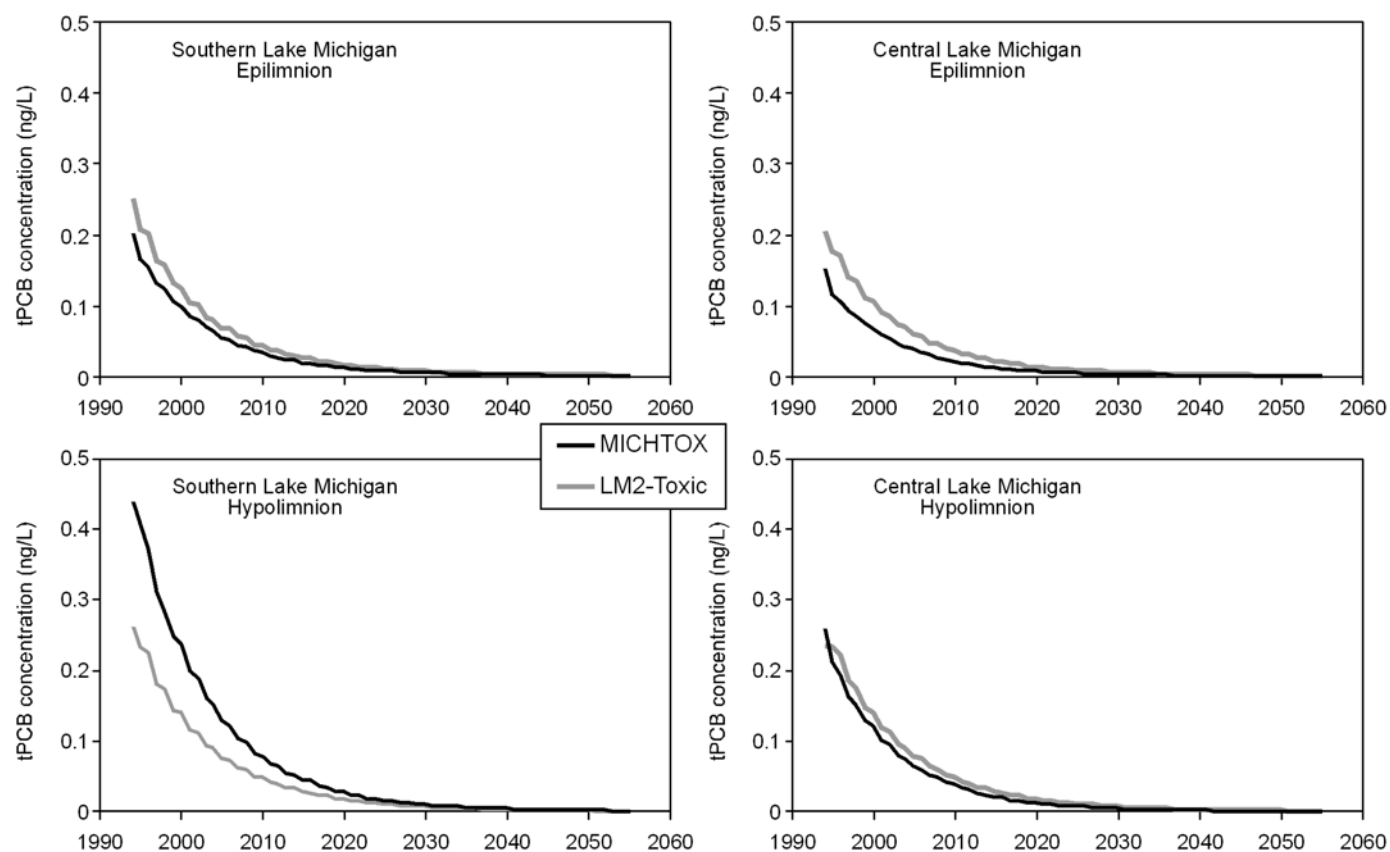

Figure 6.5. Comparison of model output annual average total PCB water concentrations for the Continued Recovery – Fast Scenario.

549

the model predictions converged over time to low concentrations. In the Constant Conditions Scenario results, differences in model parameterization resulted in differences in long-term predicted concentrations. For scenarios in which the external forcing functions declined over time, the differences in predicted concentrations were still present, but the magnitude of the difference was small compared to the overall decline in concentrations. Thus for long-term predictions, the rate of decline was more influential than differences between the model parameters.

The bioaccumulation models were also compared for the Constant Conditions Scenario and the Continued Recovery – Fast Scenario. For the Constant Conditions Scenario, MICHTOX predicted lower total PCB concentrations than LM Food Chain in the 5-6 year-old lake trout at both locations (Figure 6.6). The predicted concentration differences were larger for the central Lake Michigan/Sturgeon Bay results than the southern Lake Michigan/Saugatuck results. Differences in lake trout concentrations predicted by the models were a function of both the exposure concentrations predicted by the water quality models and factors affecting bioaccumulation in the food chain models.

The results from the bioaccumulation models for the Continued Recovery – Fast Scenario (Figure 6.7)

were similar to the results from the fate and transport models. PCB concentrations declined over time to low concentrations, with the difference in predicted concentrations between the models becoming smaller over time. For Saugatuck, the LM Food Chain model predicted that the 0.075 µg/g lake trout PCB concentration target would be achieved in 2033, and the MICHTOX food chain submodel predicted it would be achieved in 2025. For Sturgeon Bay, the LM Food Chain predicted a much slower decline than the MICHTOX food chain submodel, with the target being reached in 2036 and 2018, respectively. The difference in time required to achieve the target concentration was primarily due to the delay in the start of the concentration decline in the LM Food Chain predictions.

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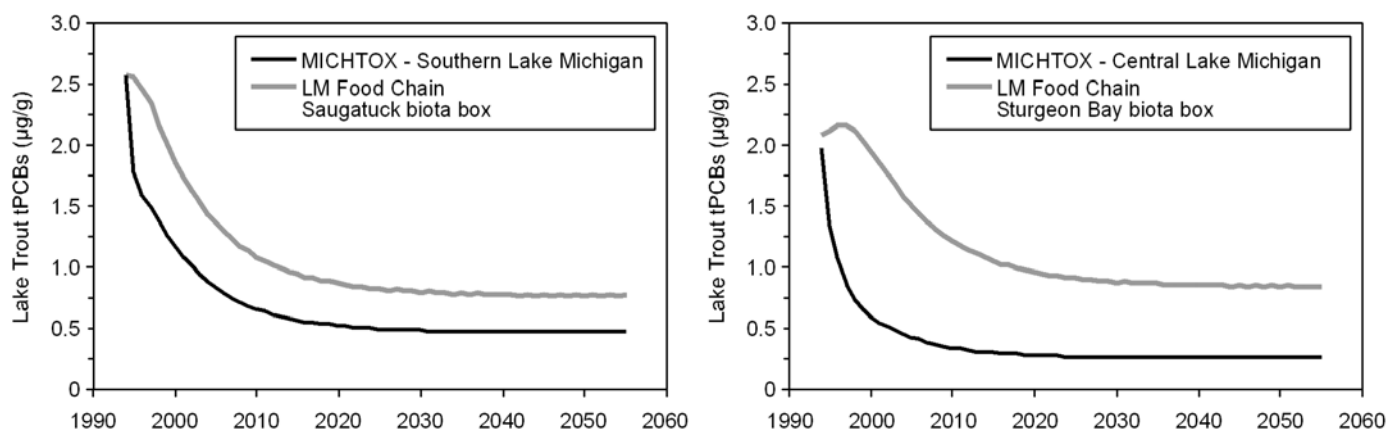
Figure 6.6. Comparison of the bioaccumulation model annual average total PCB concentration results for the Constant Conditions Scenario.
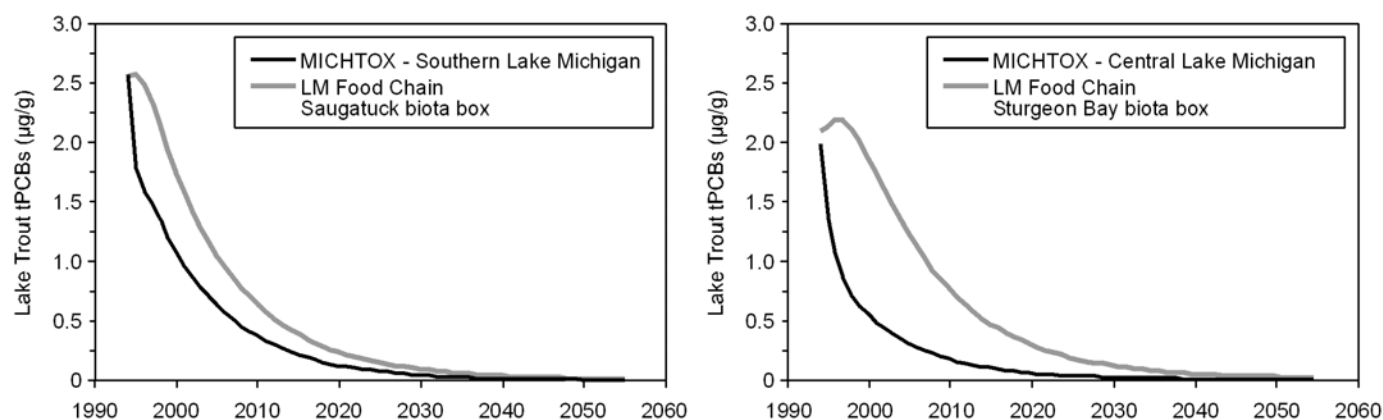
Figure 6.7. Comparison of the bioaccumulation model annual average total PCB concentration results for the Continued Recovery – Fast Scenario.

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